Guanidine, N,N"'-(iminodi-8,1-octanediyl)bis-13516-27-3 | DTXSID7042015

13516-27-3 DTXSID7042015	

Model Performance

Model	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 89.6

Global applicability domain: Outside

Local applicability domain index: 2.11e-01

Confidence level: 6.32e-01

Nearest Neighbors from the Training Set

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Tris(2-butoxyethyl) phosphate

Measured: 5.75 **Predicted:** 6.32

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Tributyl phosphate Measured: 29.5 Predicted: 29.5

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Dibutyl phthalate Measured: 166 Predicted: 14.2

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Di(2-ethylhexyl) phthalate

Measured: 589 Predicted: 295

Image not found

N-(2-Ethylhexyl)-1-isopropyl-4-methylbiclyclo[2:2:2]oct-5-ene-

2,3-dicarboximide Measured: 933 Predicted: 656